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Thermodynamics of the Antiviral and Antiparkinsonian Drug Amantadine Hydrochloride: Condensed State Properties and Decomposition

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Abstract

© 2017 American Chemical Society. Heat capacities of the antiviral and antiparkinsonian drug amantadine hydrochloride in the crystalline state were measured by adiabatic and differential scanning calorimetry in the temperature range from 5 K to 470 K. Two unresolved low-enthalpy solid-to-solid phase transitions with peak maxima at 120.0 K and 123.1 K were detected. Thermodynamic functions for crystalline amantadine hydrochloride were derived from the data obtained. Decomposition of amantadine hydrochloride was studied by the Knudsen effusion method. Quantum chemical calculations supported completeness of the amantadine hydrochloride ionic pair disintegration under the effusion conditions. A data treatment model considering the difference in effusion rates of the decomposition products, anisotropy failure in the vicinity of the orifice, and vapor undersaturation in the effusion cell was developed. Thermodynamic parameters for the decomposition were thus derived and shown to be consistent with available literature data on decomposition of similar organic hydrochlorides and with the entropy of reaction calculated directly from the entropies of the decomposition reaction participants. The obtained set of thermodynamic properties of the medication is expected to provide new key information necessary for optimization of production and storage conditions. (Graph Presented).

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References

[1] Bagrii, E. I. Adamantanes: Production, properties, application; Nauka: Moscow, 1989, [in Russian].

[2] Morozov, I. S.; Petrov, V. I.; Sergeeva, S. A. Pharmacology of Adamantanes; Volgograd Medical Academy: Volgograd, 2001, [in Russian].

[3] Oxford, J. S.; Galbraith, A. Antiviral activity of amantadine: a review of laboratory and clinical data Pharmacol. Ther. 1980, 11, 181-262 10.1016/0163-7258(80)90072-8

[4] De Clercq, E. Antiviral drugs in current clinical use J. Clin. Virol. 2004, 30, 115-133 10.1016/j.jcv.2004.02.009

[5] Morozov, I. S.; Ivanova, I. A.; Lukicheva, T. A. Actoprotector and Adaptogen Properties of Adamantane Derivatives (A Review) Pharm. Chem. J. 2001, 35, 235-238 10.1023/A:1011905302667

[6] Amantadine hydrochloride: https://www.ncbi.nlm.nih.gov/medgen/181680 (accessed on December 20, 2016).

[7] Bazyleva, A. B.; Blokhin, A. V.; Kabo, A. G.; Kabo, G. J.; Emel'yanenko, V. N.; Verevkin, S. P. Thermodynamic properties of 1-aminoadamantane J. Chem. Thermodyn. 2008, 40, 509-522 10.1016/j.jct.2007.08.002

[8] Gobble, C.; Rath, N.; Chickos, J. The Vaporization Enthalpies and Vapor Pressures of Some Primary Amines of Pharmaceutical Importance by Correlation Gas Chromatography J. Chem. Eng. Data 2013, 58, 2600-2609 10.1021/je400498a

[9] Harvey, P. D.; Gilson, D. F. R.; Butler, I. S. A study of the phase transition and molecular motion in adamantanamine hydrochloride J. Phys. Chem. 1987, 91, 1267-1270 10.1021/j100289a046

[10] Bélanger-Gariépy, F.; Brisse, F.; Harvey, P. D.; Butler, I. S.; Gilson, D. F. R. Structure of adamantanamine hydrochloride at 143 K Acta Crystallogr., Sect. C: Cryst. Struct. Commun. 1987, C43, 756-759 10.1107/S010827018709423X

[11] Parsonage, N. G.; Staveley, L. A. K. Disorder in Crystals; Clarendon Press: Oxford, 1978.

[12] Lasocha, B.; Gawel, B.; Lasocha, W. Powder diffraction investigations of some organic hydrochlorides Powder Diffr. 2006, 21, 310-313 10.1154/1.2383064

[13] Meija, J.; Coplen, T. B.; Berglund, M.; Brand, W. A.; De Bièvre, P.; Gröning, M.; Holden, N. E.; Irrgeher, J.; Loss, R. D.; Walczyk, T.; Prohaska, T. Atomic weights of the elements 2013. IUPAC Technical Report Pure Appl. Chem. 2016, 88, 265-291 10.1515/pac-2015-0305

[14] Blokhin, A. V.; Paulechka, Y. U.; Kabo, G. J. Thermodynamic Properties of [Cmim][NTf] in the Condensed State J. Chem. Eng. Data 2006, 51, 1377-1388 10.1021/je060094d

[15] Archer, D. G. Thermodynamic Properties of Synthetic Sapphire (α-AlO), Standard Reference Material 720 and the Effect of Temperature-Scale Differences on Thermodynamic Properties J. Phys. Chem. Ref. Data 1993, 22, 1441-1453 10.1063/1.555931

[16] Höhne, G. W. H.; Cammenga, H. K.; Eysel, W.; Gmelin, E.; Hemminger, W. The temperature calibration of scanning calorimeters Thermochim. Acta 1990, 160, 1-12 10.1016/0040-6031(90)80235-Q

[17] Gmelin, E.; Sarge, St. M. Calibration of differential scanning calorimeters Pure Appl. Chem. 1995, 67, 1789-1800 10.1351/pac199567111789

[18] Bazyleva, A.; Fulem, M.; Becerra, M.; Zhao, B.; Shaw, J. M. Phase Behavior of Athabasca Bitumen J. Chem. Eng. Data 2011, 56, 3242-3253 10.1021/je200355f

[19] Zaitsau, Dz.; Kabo, G. J.; Kozyro, A. A.; Sevruk, V. M. The effect of the failure of isotropy of a gas in an effusion cell on the vapor pressure and enthalpy of sublimation for alkyl derivatives of carbamide Thermochim. Acta 2003, 406, 17-28 10.1016/S0040-6031(03)00231-4

[20] Zaitsau, Dz. H.; Verevkin, S. P.; Paulechka, Y. U.; Kabo, G. J.; Sevruk, V. M. Comprehensive Study of Vapor Pressures and Enthalpies of Vaporization of Cyclohexyl Esters J. Chem. Eng. Data 2003, 48, 1393-1400 10.1021/je025634v

[21] Zaitsau, D. H.; Kabo, G. J.; Strechan, A. A.; Paulechka, Y. U.; Tschersich, A.; Verevkin, S. P.; Heintz, A. Experimental Vapor Pressures of 1-Alkyl-3-methylimidazolium Bis(trifluoromethylsulfonyl)imides and a Correlation Scheme for Estimation of Vaporization Enthalpies of Ionic Liquids J. Phys. Chem. A 2006, 110, 7303-7306 10.1021/jp060896f

[22] McQuarrie, D. A. Statistical thermodynamics; Harper and Row: New York, 1973.

[23] Neese, F. The ORCA program system Wiley Interdiscip. Rev.: Comput. Mol. Sci. 2012, 2, 73-78 10.1002/wcms.81

[24] Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian 09, Revision D.01; Gaussian Inc.: Wallingford, CT, 2013.

[25] van Alsenoy, C. Ab initio calculations on large molecules: The multiplicative integral approximation J. Comput. Chem. 1988, 9, 620-626 10.1002/jcc.540090607

[26] Feyereisen, M.; Fitzgerald, G.; Komornicki, A. Use of approximate integrals in ab initio theory. An application in MP2 energy calculations Chem. Phys. Lett. 1993, 208, 359-363 10.1016/0009-2614(93)87156-W

[27] Weigend, F.; Häser, M. RI-MP2: first derivatives and global consistency Theor. Chem. Acc. 1997, 97, 331-340 10.1007/s002140050269

[28] Weigend, F.; Ahlrichs, R. Balanced basis sets of split valence, triple zeta valence and quadruple zeta valence quality for H to Rn: Design and assessment of accuracy Phys. Chem. Chem. Phys. 2005, 7, 3297-3305 10.1039/b508541a

[29] Riplinger, C.; Neese, F. An efficient and near linear scaling pair natural orbital based local coupled cluster method J. Chem. Phys. 2013, 138, 034106 10.1063/1.4773581

[30] Liakos, D. G.; Sparta, M.; Kesharwani, M. K.; Martin, J. M. L.; Neese, F. Exploring the Accuracy Limits of Local Pair Natural Orbital Coupled-Cluster Theory J. Chem. Theory Comput. 2015, 11, 1525-1539 10.1021/ct501129s

[31] Liakos, D. G.; Neese, F. Is It Possible To Obtain Coupled Cluster Quality Energies at near Density Functional Theory Cost? Domain-Based Local Pair Natural Orbital Coupled Cluster vs Modern Density Functional Theory J. Chem. Theory Comput. 2015, 11, 4054-4063 10.1021/acs.jctc.5b00359

[32] Grimme, S.; Ehrlich, S.; Goerigk, L. Effect of the damping function in dispersion corrected density functional theory J. Comput. Chem. 2011, 32, 1456-1465 10.1002/jcc.21759

[33] Merrick, J. P.; Moran, D.; Radom, L. An Evaluation of Harmonic Vibrational Frequency Scale Factors J. Phys. Chem. A 2007, 111, 11683-11700 10.1021/jp073974n

[34] Wahlbeck, P. G. Effusion. VII. The failure of isotropy of a gas in an effusion cell and the transition region J. Chem. Phys. 1971, 55, 1709-1715 10.1063/1.1676300

[35] Wey, S. J.; Wahlbeck, P. G. Effusion IX. Application of the Failure-of-Isotropy Theory for the Effusion of Gaseous Mixtures J. Chem. Phys. 1972, 57, 2937-2939 10.1063/1.1678687

[36] Pappu, R. V.; Hart, R. K.; Ponder, J. W. Analysis and Application of Potential Energy Smoothing for Global Optimization J. Phys. Chem. B 1998, 102, 9725-9742 10.1021/jp982255t

[37] Haynes, W. M. CRC Handbook of Chemistry and Physics, 93 rd ed.; CRC Press: Boca Raton, FL, 2012.

[38] Nesmeyanov, A. N. Vapor Pressure of the Elements; Academic Press: New York, 1963.

[39] Bazyleva, A. B.; Blokhin, A. V.; Kabo, G. J.; Kabo, A. G.; Sevruk, V. M. Thermodynamic properties of 2-adamantanone in the condensed and ideal gaseous states Thermochim. Acta 2006, 451, 65-72 10.1016/j.tca.2006.08.018

[40] Clarke, E. C. W.; Glew, D. N. Evaluation of thermodynamic functions from equilibrium constants Trans. Faraday Soc. 1966, 62, 539-547 10.1039/tf9666200539

[41] Cox, J. D.; Wagman, D. D.; Medvedev, V. A. CODATA Key Values for Thermodynamics; Hemisphere Publishing Corp.: New York, 1989.

[42] Pedley, J. B. Thermochemical Data and Structures of Organic Compounds, Vol. 1; Thermodynamic Research Center: College Station, TX, 1994.

[43] Steele, W. V. The standard enthalpies of formation of cyclohexylamine and cyclohexylamine hydrochloride J. Chem. Thermodyn. 1979, 11, 1185-1188 10.1016/0021-9614(79)90112-5